

butyl 1-naphthoate
3007-95-2 | DTXSID10289046

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 53.9

Global applicability domain: Inside

Local applicability domain index: 4.86e-01

Confidence level: 6.70e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Isoamyl ether</div> <div>Measured: 170</div> <div>Predicted: 137</div>	<div>Image not found</div> <div>N,N-Diethylaniline</div> <div>Measured: 102</div> <div>Predicted: 12.8</div>	<div>Image not found</div> <div>Isoproc carb</div> <div>Measured: 8.91</div> <div>Predicted: 13.6</div>
<div>Image not found</div> <div>Menthol</div> <div>Measured: 10.8</div> <div>Predicted: 23.5</div>	<div>Image not found</div> <div>(1R,2S,5R)-(-)-Menthol</div> <div>Measured: 10.8</div> <div>Predicted: 23.5</div>	<div>Image not found</div> <div>1-Naphthalenamine, N-ethyl-</div> <div>Measured: 209</div> <div>Predicted: 47.9</div>